

What is claimed is:

1. A computer-based method of generating a quantitative structure activity relationship comprising:
 - a) calculating a numerical representation of molecules consisting of n numbers per molecule; and,
 - b) estimating a probability distribution that a said molecules is active.
2. A method as recited in claim 1, wherein:
 - a) said estimating step is calculated with Bayes Theorem.
- 10 3. A method as recited in claim 1, wherein:
 - a) said probability distribution of said estimating step comprises n one-dimensional distributions.
4. A method as recited in claim 1, wherein:
 - a) said estimating step is performed by using a means to remove linear correlations between said n numbers per molecule.
- 15 5. A method as recited in claim 4, wherein:
 - a) said means to remove linear correlations between said n numbers per molecule is a principal components analysis.

6. A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said n numbers per molecule is a matrix diagonalization.

7. A method as recited in claim 1, wherein:

5 a) said estimating step is performed by using a means to remove dependencies between said n numbers per molecule.

8. A method as recited in claim 7, wherein:

a) said means to remove dependencies between said n numbers per molecule is a principal components analysis.

10 9. A method as recited in claim 7, wherein:

a) said means to remove dependencies between said n numbers per molecule is a matrix diagonalization.

10. A method as recited in claim 1, wherein:

15 a) said estimating step is performed by estimating a distribution over a single number.

11. A method as recited in claim 1, wherein:

a) said estimating step is performed by replacing a single observation with a Gaussian distribution.